Butanamide, 4-hydroxy-927-60-6 | DTXSID5061297

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: -2.97

Global applicability domain: Inside

Local applicability domain index: 5.62e-01

Confidence level: 5.26e-01

Nearest Neighbors from the Training Set

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L-Glutamic acid Measured: -3.69 Predicted: -3.45 Image not found

L-Aspartic acid Measured: -3.89 Predicted: -3.52 Image not found

4-Aminobutanoic acid Measured: -3.17 Predicted: -2.84

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beta-Alanine Measured: -3.05 Predicted: -3.07 Image not found

Propanamide

Measured: -0.660

Predicted: -0.909